Surface and Overlayer Electronic Structure of Wide Band Gap Nitride Semiconductors

Kevin E. Smith, Boston University, DMR-9986099

The goal of this program is to measure the electronic structure of thin film wide band gap nitride semiconductors and to understand how this structure effects the growth of these nitride films, the growth of contact overlayers on the nitrides, and the chemical stability of the films and overlayers. These materials have numerous potential applications in optoelectronic and high temperature devices. Despite much study over the last decade, much remains unknown about their fundamental physical properties.

A highlight of our 2002/2003 program was the first the direct measurement of the elementally specific O *2p* and N *2p* valence and conduction band partial densities of states for an ultrathin SiO_xN_y layer High resolution soft x-ray emission (SXE) and soft x-ray absorption (SXA) spectroscopies were used to make the measurements. Experiments were performed at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory. Figure 1 shows the occupied and unoccupied states of oxygen character in SiON and pure SiO_2. The band gap for these states is identical in both materials: 8.8 eV Figure 2 shows the measurement of the nitrogen states in SiON and reveals that the band gap is much smaller: 5 eV. For more details, please see J. Appl. Phys. **94**, 3919 (2003).

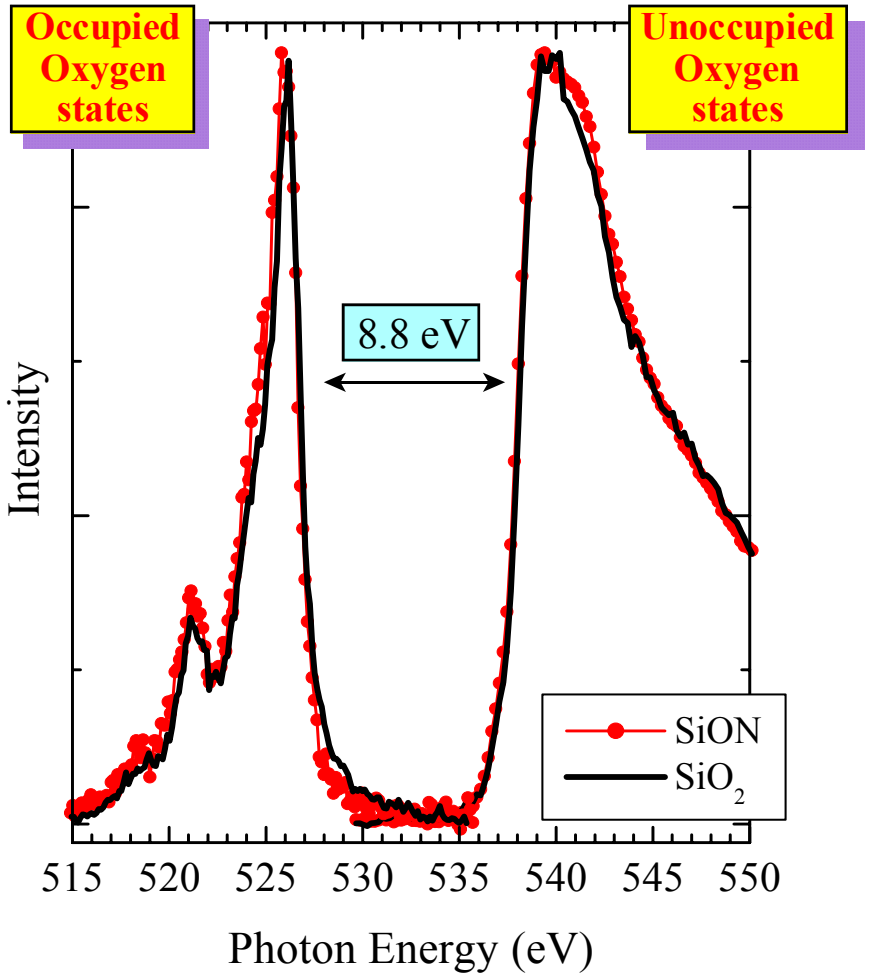

Figure 1: Occupied and unoccupied oxygen states from SiON and SiO_2; note the identical band gap of 8.8 eV for both materials.

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Educational Activities:

This program involves one undergraduate student (Paul Sheridan), two graduate students (Dongfeng Fu and James Downes) and one postdoctoral research associate (Dr. Cormac McGuinness). *Note also that the PI serves as the first Academic Director of the Center for Excellence in Teaching at Boston University. Furthermore, the PI was named the 2001 Massachusetts Professor of the Year by the Carnegie Foundation.*

Infrastructure Impact:

The PI used the present NSF award to leverage significant funds for scientific infrastructure enhancement. He was awarded $220,000 from the Defense University Research Instrumentation Program of the Army Research Office to construct a multi-technique spectrometer system to be used in this NSF program. The new system is fully operational and features both a high resolution angle resolved photoemission spectrometer (100 mm Scienta), and our novel high resolution soft x-ray emission spectrometer that was used to make the measurements presented in Figs. 1 and 2.

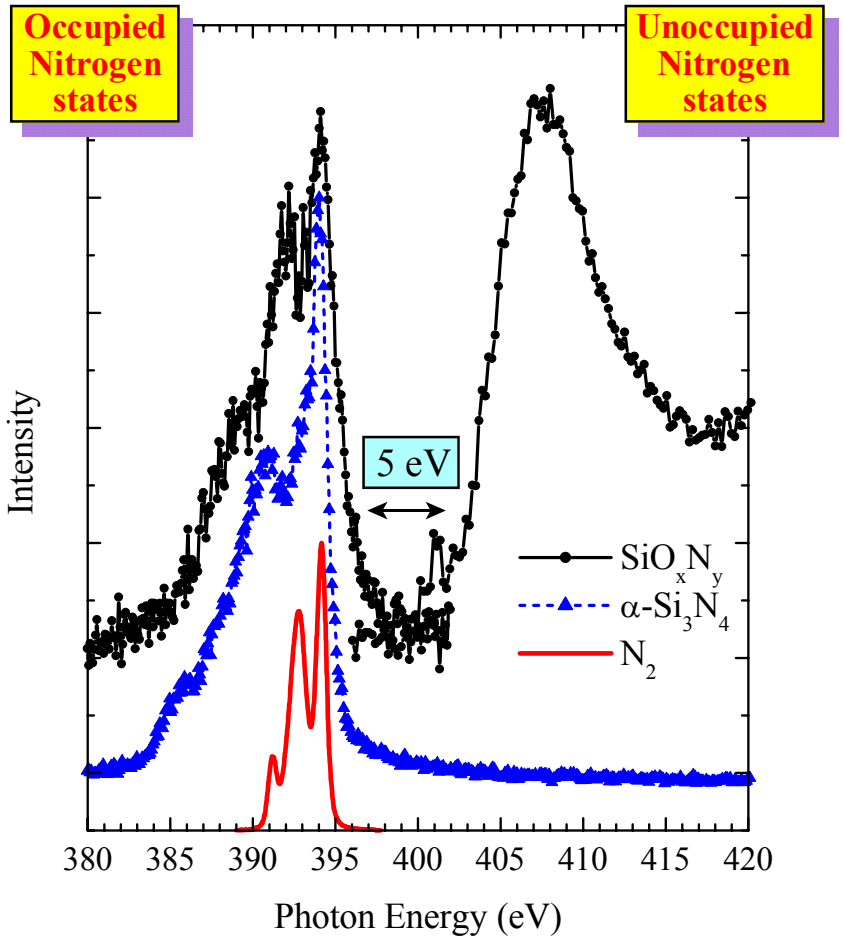

Figure 2: Occupied and unoccupied nitrogen states in SiON. Si_3N_4 and N_2 are shown for comparison.